

```
ring nodes:
```

1 2 3 4 5 6 7 8 9 10 11

ring bonds :

1-6 1-11 2-3 2-11 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

1-6 1-11 2-3 2-11 3-4 4-5

normalized bonds :

5-6 5-7 6-10 7-8 8-9 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

=> d his

(FILE 'HOME' ENTERED AT 15:42:01 ON 08 FEB 2006)

FILE 'REGISTRY' ENTERED AT 15:42:09 ON 08 FEB 2006

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3

L5 41 S L3 SSS FUL

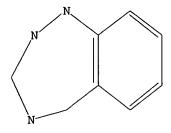
FILE 'CAPLUS' ENTERED AT 15:43:28 ON 08 FEB 2006

L6 4 S L5

=> d 13

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:203177 CAPLUS

DOCUMENT NUMBER: 140:235731

TITLE: Preparation of cinnolines and their use as

beta-lactamase inhibitors and antibacterial agents

INVENTOR(S):

PATENT ASSIGNEE(S):

SOURCE:

Musicki, Branislav

Aventis Pharma SA, Fr.
Fr. Demande, 67 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

					KIND		DATE		APPLICATION NO.								
FR					A1 2		20040312		FR 2002-10957								
WO	2004022563				A1 200			040318			WO 2003-FR2639				200309		
	W:	ΑE,	AG,	AL,	ΑU,	BA,	BB,	BR,	ΒZ,	CA,	CN,	co,	CR,	CU,	DM,	DΖ,	EC,
		GD,	GE,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KP,	KR,	LC,	LK,	LR,	LT,	LV,
		MA,	MG,	MK,	MN,	MX,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	RO,	SC,	SG,	SY,
		TN,	TT,	UA,	UZ,	VC,	VN,	ΥU,	ZA								
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪG,	ZM,	ZW,	AM,	ΑZ,	BY,
		KG,	KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
US	US 2004097490				A1 20040520				US 2003-655364					20030904			
EP	? 1537117				A1 20050608			EP 2003-769564					20030904				
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	ΑL,	TR,	BG,	CZ,	EE,	HU,	SK	
JP 2006501258				Т2		20060112			JP 2004-533566				20030904				
PRIORITY APPLN. INFO.:										FR 2	2002-	1095	7	1	A 2	0020	905
											2003-						
OTHER S	MARPAT 140:235731																

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [wherein Y = (CH2)n; n = 1 or 2; R1 = H, alkyl, (CH2)mR'; AB m = o or 1; R' = heteroaryl/aryl; R2 = H, halo, alkyl, OH and derivs., NO2, alkylaminocarbonyl/alkylsulfonyl/alkylcarbonylmonoalkyl/dialkyl/amino , alkylaminocarbonyl, alkylaminosulfonyl, CO2H and derivs., CN, alkylsulfonyloxy, alkylcarbonyl, alkyl; X = -C(:0)-N(OH)- and derivs.] were prepared as beta-lactamase inhibitors and antibacterial agents. For example, II was prepared by cyclization of 2-acetylaniline in the presence of NaNO2/HCl, oxidation of cinnolinol, mono-Boc protection at the 2-position, oximation of cinnolinone with O-(allyl)hydroxyamine, reduction of the O-alkylated oxime, Boc-deprotection, and cyclization of III-2HCl with diphosquee in the presence.of MeCN/TEA/DMAP. Selected I were able to inhibit either TEM-1 (enzyme from Escherichia coli) and P99 (enzyme from E. Cloacae) with IC50 values in the range of 0.012 mM to 0.57 mM and 0.015 to 0.46 mM, resp., when tested in competition expts. using nitrocefin as the reporter substrate. I were tested against two Gram-pos. bacteria as well as four Gram-neg. bacteria. Thus, I are and their compns. with β -lactam antibiotics, are useful as beta-lactamase inhibitors and

GI

antibacterial agents.

IT 667467-63-2P 667467-74-5P, 2-Propenyl [(3-oxo-2,3,4,5-tetrahydro-2,5-methano-1H-1,2,4-benzotriazepin-4yl)oxy]acetate 667467-79-0P 667467-82-5P 667467-85-8P 667467-88-1P 667467-91-6P 667467-92-7P 667467-93-8P 667468-03-3P 667468-04-4P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (antibacterial agent; preparation of cinnolines as beta-lactamase inhibitors and anti-bacterial agents) 667467-63-2 CAPLUS RN

2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-4-(2-CN propenyloxy) - (9CI) (CA INDEX NAME)

RN 667467-74-5 CAPLUS

Acetic acid, [(1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-CN yl)oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
H \\
N \\
N \\
O \\
O \\
CH_2 - C - O - CH_2 - CH = CH_2
\end{array}$$

RN 667467-79-0 CAPLUS

Acetic acid, [[1,5-dihydro-1-(methylsulfonyl)-3-oxo-2,5-methano-2H-1,2,4-CN benzotriazepin-4(3H)-yl]oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)

RN 667467-82-5 CAPLUS

CN Acetic acid, [[1-[(benzoylamino)carbonyl]-1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)

RN 667467-85-8 CAPLUS

CN Acetic acid, [[1,5-dihydro-3-oxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, 2-propenyl ester (9CI) (CA INDEX NAME)

RN 667467-88-1 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydroα,3-dioxo-4-[2-oxo-2-(2-propenyloxy)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 667467-91-6 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 667467-92-7 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-methyl-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667467-93-8 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-4-(2-propenyloxy)-1-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

$$CH_2$$
 N
 N
 N
 N
 N
 N
 $O-CH_2-CH=CH_2$

RN 667468-03-3 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 667468-04-4 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

IT 667467-70-1P 667467-80-3P 667467-81-4P 667467-83-6P 667467-84-7P 667467-86-9P 667467-87-0P 667467-89-2P 667467-90-5P 667467-94-9P 667467-95-0P 667467-96-1P 667467-97-2P 667467-98-3P 667467-99-4P 667468-00-0P 667468-01-1P 667468-02-2P

CN

667468-05-5P 667468-06-6P 667468-07-7P 667468-08-8P 667468-09-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antibacterial agent; preparation of cinnolines as beta-lactamase inhibitors and anti-bacterial agents)

RN 667467-70-1 CAPLUS

2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 667467-80-3 CAPLUS

CN Acetic acid, [[1,5-dihydro-1-(methylsulfonyl)-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]- (9CI) (CA INDEX NAME)

RN 667467-81-4 CAPLUS

CN Acetic acid, [[1,5-dihydro-1-(methylsulfonyl)-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-80-3 CMF C12 H13 N3 O6 S

CM 2

CRN 108-18-9 CMF C6 H15 N

i-Pr-NH-Pr-i

667467-83-6 CAPLUS RN

Acetic acid, [[1-[(benzoylamino)carbonyl]-1,5-dihydro-3-oxo-2,5-methano-2H-CN 1,2,4-benzotriazepin-4(3H)-yl]oxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O & O \\
 & \parallel & \parallel \\
 & Ph-C-NH-C \\
\hline
 & N & N \\
 & O-CH_2-CO_2H
\end{array}$$

RN

667467-84-7 CAPLUS
Acetic acid, [[1-[(benzoylamino)carbonyl]-1,5-dihydro-3-oxo-2,5-methano-2H-CN 1,2,4-benzotriazepin-4(3H)-yl]oxy]-, compd. with N-(1-methylethyl)-2propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-83-6 CMF C19 H16 N4 O6 10/655,364

CM 2

CRN 108-18-9 CMF C6 H15 N

i-Pr-NH-Pr-i

RN

667467-86-9 CAPLUS Acetic acid, [[1,5-dihydro-3-oxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5-CN methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]- (9CI) (CA INDEX NAME)

RN 667467-87-0 CAPLUS

CN Acetic acid, [[1,5-dihydro-3-oxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5methano-2H-1,2,4-benzotriazepin-4(3H)-yl]oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-86-9 CMF C18 H16 N4 O7 S

CM 2

CRN 108-18-9 CMF C6 H15 N

i-Pr-NH-Pr-i

RN

667467-89-2 CAPLUS Acetic acid, [(1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)-CN yl)oxy]- (9CI) (CA INDEX NAME)

667467-90-5 CAPLUS RN

CN Acetic acid, [(1,5-dihydro-3-oxo-2,5-methano-2H-1,2,4-benzotriazepin-4(3H)yl)oxy]-, compd. with N-(1-methylethyl)-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 667467-89-2 CMF C11 H11 N3 O4

CM 2

CRN 108-18-9 CMF C6 H15 N

i-Pr-NH-Pr-i

RN 667467-94-9 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, 1,3,4,5-tetrahydro-3-oxo-N-(phenylsulfonyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667467-95-0 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, N-benzoyl-1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \circ & \circ \\
 & \parallel & \parallel \\
 & Ph-C-NH-C
\end{array}$$

$$\begin{array}{c|c}
 & N & \bullet \\
 & N & \bullet \\
 & O-CH_2-CH=CH_2
\end{array}$$

RN 667467-96-1 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro- α ,3-dioxo-4-(2-propenyloxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 667467-97-2 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-sulfonamide, 1,3,4,5-tetrahydro-N-methyl-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667467-98-3 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carbothioamide, 1,3,4,5-tetrahydro-3-oxo-N-phenyl-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667467-99-4 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-(methylsulfonyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667468-00-0 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 N
 $O-CH_2-CH=CH_2$

RN 667468-01-1 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-carboxamide, 1,3,4,5-tetrahydro-3-oxo-N-(phenylmethyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667468-02-2 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-(phenylmethyl)-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667468-05-5 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetamide, 1,3,4,5-tetrahydro-3-oxo-4-(2-propenyloxy)- (9CI) (CA INDEX NAME)

RN 667468-06-6 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(sulfooxy)-, α-ethyl ester, sodium salt (9CI) (CA INDEX NAME)

Na

RN 667468-07-7 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-methyl-4-(sulfooxy)-, sodium salt (9CI) (CA INDEX NAME)

Na

RN 667468-08-8 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepin-3(1H)-one, 4,5-dihydro-1-(3-pyridinylmethyl)-4-(sulfooxy)-, sodium salt (9CI) (CA INDEX NAME)

● Na

RN 667468-09-9 CAPLUS

CN 2,5-Methano-2H-1,2,4-benzotriazepine-1-acetic acid, 1,3,4,5-tetrahydro-3-oxo-4-(sulfooxy)-, α -ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:77053 CAPLUS

DOCUMENT NUMBER: 112:77053

TITLE: Thermally induced fragmentation and cyclization of

C-azidohydrazones

AUTHOR(S): Bruche, Luca; Garanti, Luisa; Zecchi, Gaetano

CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milan, Milan, 20133, Italy

SOURCE: Journal of Heterocyclic Chemistry (1989), 26(3),

619-24

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:77053

GI

AB C-Azidohydrazones RNHN:CR1CO2R2 (I, R = Ph, 4-MeC6H4, 3,5-Me2C6H3, 2,6-Me2C6H3, 2-MeC6H4, R2 = Me; R = 2-NCC6H4, R2 = Et; R1 = N3) were synthesized from the corresponding C-chlorohydrazones I (R, R2 = same; R1 = C1) and submitted to thermal decomposition in boiling C6H6. Various kinds of products were obtained due to competitive modes of evolution of first-formed nitrenes I (R1 = N•), namely H abstraction to form aminohydrazones I (R1 = NH2) and benzotriazepine II and radical fragmentation to give diaryls RPh and arylglyoxylate arylhydrazones RNHN:CRCO2R2. Ring-closed products, namely 1,2,4-triazoles III and imidazolones IV were also formed.

IT 125240-53-1P

RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in thermal decomposition of azidohydrazone)

RN 125240-53-1 CAPLUS

CN 1H-1,2,4-Benzotriazepine-3-carboxylic acid, 2,5-dihydro-9-methyl-, methyl ester (9CI) (CA INDEX NAME)

10/655,364

ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:75084 CAPLUS

DOCUMENT NUMBER: 94:75084

TITLE: Crystal structure of 1,3-diphenyl-5-

carbethoxymethylene-1H-4,5-dihydro-1,2,4-

benzotriazepine

AUTHOR(S): Perez-Salazar, A.; Cano, F. H.; Garcia-Blanco, S. CORPORATE SOURCE: Inst. Quim. Fiz. "Rocasolano", CSIC, Madrid, 6, Spain SOURCE: Journal of Crystal and Molecular Structure (1980),

Volume Date 1979, 9(6), 317-23 CODEN: JCMLB5; ISSN: 0308-4086

DOCUMENT TYPE: Journal LANGUAGE: English

AB The title compound is orthorhombic, space group P212121, with a 15.1342(3), b 14.1692(3), and c 9.6533(3) Å; d.(exptl.) = 1.23 and Z = 4. The structure was solved by direct methods and refined to R 0.048 (Rw = 0.068) for 1831 observed reflections. An intramol. H bond is present. The conformation of the 7-membered ring is boatlike with a quasi-mirror plane through N(1).

IT 76553-23-6

RL: PRP (Properties)
(crystal structure of)

RN 76553-23-6 CAPLUS

CN Acetic acid, (1,2-dihydro-1,3-diphenyl-5H-1,2,4-benzotriazepin-5-ylidene), ethyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

10/655,364

ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:198370 CAPLUS

DOCUMENT NUMBER: 92:198370

TITLE: Studies on 7-membered benzo condensed heterocycles.

6. 5-0xo-1H-4,5-dihydro-1,2,4-benzotriazepines. Chemical behavior towards alkylating, acidic and

alkaline agents

AUTHOR(S): Bianchi, Mario; Hausermann, Enrico; Rossi, Silvano

CORPORATE SOURCE: Dep. Chem., Roussel Maestretti S.p.A., Milan, 20131,

Italy

SOURCE: Journal of Heterocyclic Chemistry (1979), 16(7),

1411-16

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 92:198370

AB The chemical behavior of 4-methyl- and 4-phenyl-5-oxo-1H-4,5-dihydro-1,2,4-benzotriazepines towards methylating and acidic agents was studied. The

4-Me derivative, when treated with FSO3Me furnished, after crystallization

from H2O, a

quaternary salt (2,4-dimethyl-5-oxo-1H-4,5-dihydro-1,2,4-benzotriazepinium fluorosulfonate); from the 4-Ph derivative a complex mixture was obtained, which, after boiling with H2O, afforded 2-methylindazolone, PhNH2.HO3SF and HCO2H. In acidic medium the 4-Me derivative isomerized to 1-imino-3-methylquinazolin-4-one, but the 4-Ph derivative exclusively yielded

products resulting from ring opening. In alkaline medium, both compds. gave

hydrolytic cleavage products.

IT 73647-13-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

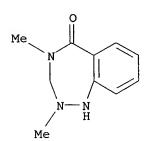
(preparation and reactions of)

RN 73647-13-9 CAPLUS

CN 1H-1,2,4-Benzotriazepinium, 4,5-dihydro-2,4-dimethyl-5-oxo-, fluorosulfate (9CI) (CA INDEX NAME)

CM 1

CRN 73647-12-8 CMF C10 H12 N3 O



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 15181-47-2 CMF F O3 S